

Nontrivial quantized Berry phases for itinerant spin liquids

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Quantized Berry phases as local order parameters in t - J models are studied. A texture pattern of the local order parameters is topologically stable due to the quantization of non-Abelian Berry phases defined by low-energy states below a spin gap, which exists in the large J/t case with a few electrons. We have confirmed that itinerant singlets in the wide class of t - J models carry the nontrivial Berry phase π . In the large J/t case for the one-dimensional t - J model, Berry phases are uniformly π when the number of electrons is $N = 4n + 2$, ($n = 0, 1, 2, \dots$).

KEYWORDS: Non-Abelian Berry phases, quantum liquids, topological orders, t - J model, strongly correlated electron

New quantum numbers have recently been proposed to classify states of matters beyond the Landau symmetry-breaking description, such as ground state degeneracy, non-Abelian Berry's phases and edge excitations.¹⁻⁴ Such a nontrivial class of matter is identified as possessing topological order, which can be useful to characterize quantum liquids; the Haldane spin chain,⁵ the valence bond solid states,⁶ and the spin-Peierls system.⁷ Also, the entanglement entropy has attracted attention,⁸ which provides a new physical insight for the gapped quantum liquids with a nontrivial topological order thorough the bulk-edge correspondence.^{9,10} Moreover, topological quantities such as the Chern numbers, which have successfully characterized the quantum Hall states¹¹ and the generic quantum liquids,^{3,4} have the advantage that these quantities are quantized, which implies they are topologically protected against small perturbations. In addition to the Chern numbers, the Berry phases can be also quantized in some situations. When the ground state is gapped and is invariant under some anti-unitary operation, the Berry phase, which takes an arbitrary real number in principle, is quantized to the two values: a trivial value 0 or a nontrivial value $\pi \pmod{2\pi}$. This scheme has been proposed and applied for gapped quantum liquids.^{12,13} Since the Berry phase is defined by a *local* $SU(2)$ twist at a specific link, the Berry phase can be used as a *local* order parameter, which does not have any classical correspondent since it is gauge dependent. Note that the expectation value of any observable is invariant under unitary transformations of bases, which means that it is a gauge invariant. In dimerized Heisenberg systems, the Berry phases break

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the translational symmetry: the Berry phases at strong bonds (or at weak bonds) are π (or zero). It implies that dimer singlets are mostly localized at the strong bonds. The scheme can be applied to the strongly correlated electron system as well.¹² To take an advantage of topological stability against small perturbations such as randomness, a finite gap above the ground state is required. If one does not require the topological stability, a Berry phase can be obtained even if there is no finite gap.¹⁴

In the present work, the scheme to calculate the topologically stable Berry phase for a gapped system is applied to the t - J model as one of the strongly correlated systems.^{12,13} In contrast to the localized singlets in the dimerized Heisenberg systems, singlets in the t - J model are itinerant. Therefore there can be gapless charge excitations above the ground state, which implies existence of a low energy cluster of eigenstates even if the spin excitation is gapped. Then, we need to use a non-Abelian Berry connection, which is defined by all the eigenstates in the cluster.¹² The Berry phase in this case is defined by taking a trace over the eigenstates. It reminds us that the standard order parameter as an expectation value of an operator is calculated by taking a trace with the density matrix when the system is in a mixed state; besides, when the ground state is degenerate, one needs to take an average over the degenerate eigenstates at zero temperature.

The t - J model is an effective model of the large U repulsive Hubbard model, which describes the hole-doped Mott insulator. The study on two dimensional(2D) t - J models was stimulated by the discovery of high- T_c superconductivity of the copper-oxygen planes.^{15,16} In addition, one-dimensional(1D) t - J models have received much attention recently because of the common properties between 1D and 2D strongly correlated electron systems¹⁷ and, more directly, possibilities of quasi-1D superconductivity.¹⁸ Motivated this proposition, many theoretical studies on 1D t - J models were focused on superconducting states. For simplicity, we focus on the large J/t region in the paper.

The t - J model is defined on the subspace without double occupancy as

$$H = H_t + H_J, \quad (1)$$

$$H_t = \sum_{ij} t_{ij} \mathcal{P} \mathbf{c}_i^\dagger \mathbf{c}_j \mathcal{P}, \quad (2)$$

$$H_J = \sum_{ij} J_{ij} \left(\mathbf{S}_i \cdot \mathbf{S}_j - \frac{n_i n_j}{4} \right), \quad (3)$$

where $\mathbf{c}_i^\dagger = (c_{i\uparrow}^\dagger, c_{i\downarrow}^\dagger)$, $n_i = \mathbf{c}_i^\dagger \mathbf{c}_i$, $\mathbf{S}_i = \frac{1}{2} \mathbf{c}_i^\dagger \boldsymbol{\sigma} \mathbf{c}_i$ and $\boldsymbol{\sigma}$ is a vector form of the Pauli matrices. Here the operator $\mathcal{P} = \prod_i (1 - c_{i\uparrow}^\dagger c_{i\uparrow} c_{i\downarrow}^\dagger c_{i\downarrow})$ is the projection to states with no double-occupancy. In this paper, we limit ourselves to a 2D square lattice or a 1D chain under the periodic boundary condition with the lattice size L and the number of up (down) electrons $N_\uparrow (N_\downarrow)$. Hereafter, the hopping matrix t_{ij} has a non-zero value t only on nearest-neighbor links, while dimerization or next-nearest-neighbor interactions can be introduced for the spin exchange

J_{ij} . We take $t = 1$ as a unit of energy in the numerical calculations. Let us describe the method to calculate Berry phases. For a parameter-dependent Hamiltonian, $H = H(\theta)$, the Berry phase γ of an M -fold multiplet is customarily given by the $U(1)$ part of non-Abelian Berry connection as $i\gamma = \int_C \text{Tr} A(\theta)$, where the Berry connection A is the $M \times M$ matrix defined as $(A(\theta))_{mm'} = \langle \psi_m(\theta) | d | \psi_{m'}(\theta) \rangle = \langle \psi_m(\theta) | \frac{d}{d\theta} | \psi_{m'}(\theta) \rangle d\theta$ and states are normalized eigenstates of the Schrödinger equation; $H(\theta) | \psi_m(\theta) \rangle = E_m(\theta) | \psi_m(\theta) \rangle$, ($1 \leq m \leq M$).¹⁹ Note that when the M states are degenerate at $\theta = 0$ a standard order parameter at zero temperature is defined as $\langle \mathcal{O} \rangle = \sum_m \langle \psi_m(0) | \mathcal{O} | \psi_m(0) \rangle / M$ and has some analogy with the non-Abelian Berry phase. The main differences are the differentiation and the integration for the Berry phase, which lead to the gauge dependence.

The Berry phase γ is proved to be real and has ambiguity due to gauge freedom of eigenstates. To avoid it, we should fix the gauge. Following ref. 3, the gauge-fixed states can be obtained from $P | \phi_m \rangle$ with a generic basis set $| \phi_m \rangle$ and the gauge invariant projection operator P defined as $P = \sum_m | \psi_m(\theta) \rangle \langle \psi_m(\theta) |$. However, in this paper, we use another way to calculate the Berry phase by introducing a *gauge-invariant Berry phase* for the lattice analogue of the Berry connection. It is defined as follows by discretizing the parameter space of θ into K points:^{12,20}

$$\gamma = \lim_{K \rightarrow \infty} \gamma_K, \quad \gamma_K = - \sum_{k=1}^K \arg \det C(\theta_k), \quad (4)$$

where $C(\theta_k)$ is the $M \times M$ matrix defined as $(C(\theta_k))_{mm'} = \langle \psi_m(\theta_k) | \psi_{m'}(\theta_{k+1}) \rangle$ under the periodic condition: $\theta_{K+1} = \theta_1$. The Berry phase in a continuum is gauge dependent but the one defined here for the discretized parameter space is gauge invariant. The gauge invariance here means that it is invariant under gauge transformations after fixing the discretization. This Berry connection can be considered as the connection of a 1D analogue of the lattice gauge theory. Note that the periodic condition in the parameter space, $| \psi_m(\theta_{K+1}) \rangle = | \psi_m(\theta_1) \rangle$, guarantees the gauge invariance of the Berry phase here. As a generic parameter θ in the definition of the Berry phase, we use a local spin twist in the present study:

$$S_i^+ S_j^- + S_i^- S_j^+ \rightarrow e^{i\theta_{ij}} S_i^+ S_j^- + e^{-i\theta_{ij}} S_i^- S_j^+, \quad (5)$$

where $S_i^\pm = S_i^x \pm iS_i^y$. Since the Berry phase is defined by the local twist at each link ij , the Berry phase is used as a local order parameter on the link. Note that θ_{ij} is introduced only to the spin exchange terms H_J , and it does not modify the other terms in the Hamiltonian. We denote the Hamiltonian with θ_{ij} as $H(\theta_{ij})$.

The gauge-invariant Berry phase here is also quantized when the Hamiltonian $H(\theta_{ij})$ is invariant under an anti-unitary operator, i.e., $[H(\theta_{ij}), \Theta] = 0$. The anti-unitary operator in the present case is the time-reversal operator written as $\Theta = KU$ with complex conjugation K and a unitary operator defined as $U = \prod_i e^{\frac{\pi}{2}(S_i^+ - S_i^-)}$. The quantization of the K -discretized Berry phase γ_K is proved in the same way as in refs.12 and 13. Since the Berry phase is

quantized ($\gamma = 0$ or π) and is used as a link-variable as discussed above, each link has one of three labels: “0-bond”, “ π -bond”, or “undefined (or gapless)”. As a whole system, a texture pattern of the local order parameters is obtained.

Before we show the results, we comment on some technical aspects. We can obtain γ even for small K without numerical error due to the quantization of γ_K . For example, in the one singlet case ($L = 2, N_\uparrow = N_\downarrow = 1$), $K = 3$ is enough to obtain the correct value, $\gamma = \pi$, in the large K limit. On the other hand, absolute value of $\Gamma_K = \det \prod_{k=1}^K C(\theta_k)$ is used as a convenient criterion for the convergence. We have checked it for all the results shown below.

In the t - J model with a few electrons, the spin gap is finite but the charge excitation is gapless. Then, low energy states below the spin gap are treated as an M -fold multiplet to calculate the Berry phase. To understand the spin gap in a few electrons case, we consider the large J limit. For simplicity, let us consider the one singlet case, $N_\uparrow = N_\downarrow = 1$ for a while. The M -fold degenerate states below the spin gap form a multiplet, where M is equal to the number of links and the spin gap is of the order of J . These are spanned by the localized singlet states $|l\rangle$, where the link number l indicates the position of the localized singlet ($1 \leq l \leq M$). These states are bundled as a multiplet. Then, we consider the hopping process of a singlet as a perturbation in a similar way to refs. 16 and 21. In the eigenspace spanned by $|l\rangle$, the effective Hamiltonian is obtained by the second perturbation theory as

$$H_{\text{eff}} = \sum_{ll'} |l\rangle \langle l| H^{(2)} |l'\rangle \langle l'|, \quad H^{(2)} = H_t \frac{1}{E - H_J} H_t.$$

When we switch on hopping process, the singlet starts to move around with the effective hopping $t_s = \frac{t^2}{J}$. The degeneracy is lifted by $H^{(2)}$ and its bandwidth is of the order of t_s . When J/t is large enough, the spin gap above the band is stable in the thermodynamic limit, $L \rightarrow \infty$, as shown in Fig. 1. The charge gap, which is a small gap between the states in the multiplet, is of the order of t_s/M and becomes zero in the thermodynamic limit. Note that the number of the states is $M = L$ for a 1D chain or $M = 2L^2$ for a 2D square lattice. Although the degeneracy of the multiplet is macroscopic, the Berry phase of states below the spin gap is numerically stable.

Figure 2(a) shows a texture pattern for one singlet states ($N_\uparrow = N_\downarrow = 1$) in the t - J model on a 4×4 lattice under the periodic boundary condition. When the spin exchange J/t is large, a finite gap exists above the $M = 32$ states. As shown in Fig. 2(a) the uniform π -bonds are obtained. In addition, when the dimerization of the spin exchange is introduced as $J^S > J^W$, the dimerization gap opens up. The Berry phase of the states below the dimerization gap will be π for strong bonds with J^S and 0 for weak bonds with J^W . For example, as shown in Fig. 2(b), when eight links with the strong interaction are alternately distributed along the x -axis on a 4×4 lattice, the dimerization gap opens above the $M = 8$ states and the texture pattern coincides with the distribution of the strong bonds with J^S .

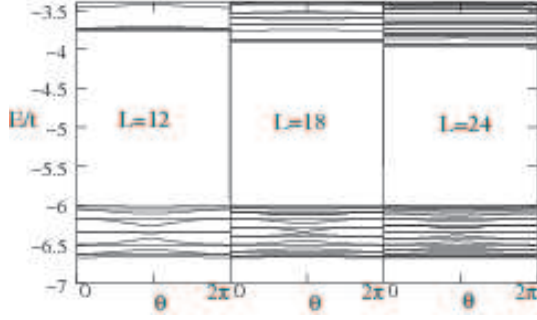


Fig. 1. Energy diagram as a function of a local spin twist θ in the 1D t - J model with $N_{\uparrow} = N_{\downarrow} = 1$ and $J/t = 6$. The system size is $L = 12, 18, 24$.

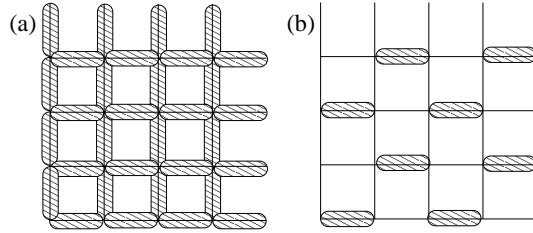


Fig. 2. A texture pattern of the local order parameters for the one singlet states ($N_{\uparrow} = N_{\downarrow} = 1$) in the t - J model on a 4×4 lattice under the periodic boundary condition. The shadowed links denote the π -bonds and the others are the 0-bonds. (a) The local order parameters for the $M = 32$ states for the t - J model with $J/t = 8$. (b) The local order parameters for the $M = 8$ states of the dimerized t - J model with the dimerization $J^S/J^W = 2$ and $J^W/t = 8$. The strong bonds with J^S correspond with the π -bonds and the other links are weak bonds with J^W .

To explain the results in Fig. 2, let us consider the perturbation from the large J/t limit in the 1D case for simplicity. In the large J/t limit, the Berry phase of the multiplet is given as a sum of respective Berry phases of the localized singlet states $|l\rangle$. Each state gives the Berry phase π only at the specific link where the singlet exists. Then the Berry phases of the multiplet are π uniformly. It does not depend on the dimensionality.

Unless the spin gap closes, any perturbation cannot modify the texture pattern of the local order parameters even if the level-crossing within the multiplet occurs. This is the topological stability of the quantized Berry phase. Then, the result at $J/t = 8$ shown in Fig. 2(a) should be the same as uniform π Berry phase in the large J/t limit, because the spin gap does not close at $J/t = 8$. In any dimension, the situation can be the same. In addition, the result shown in Fig. 2(b) is the same as in the case $J^S/t = \infty$ and $J^W/t = 0$.

It is interesting to consider the Berry phase in other t - J models. In addition to the simple t - J chain, three modifications can be of interest as spin-gapped systems at finite filling in the 1D case; (1) the dimerized t - J chain²² by putting $J_{i,i+1} = J(1 + (-1)^i \delta)$, (2) the t - J - J' chain²³ by putting $J_{i,i+1} = J, J_{i,i+2} = J'$ and (3) the t - J - V chain²⁴ by adding $H_V = V \sum_i n_i n_{i+1}$. We

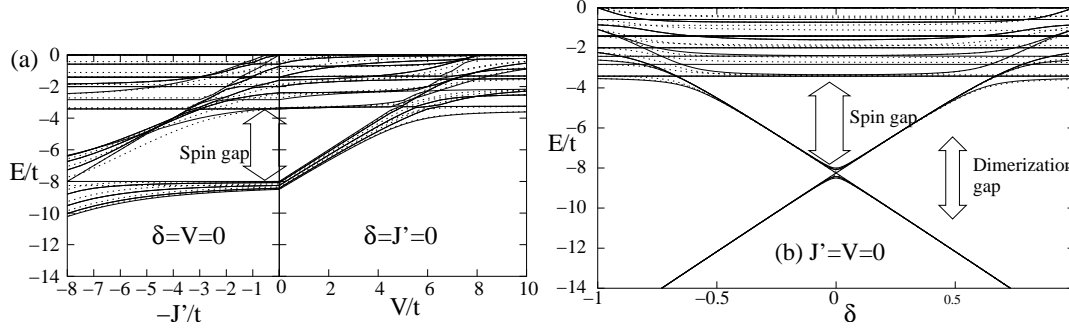


Fig. 3. Energy diagram for the 1D t - J model with $L = 8$, $J/t = 8$ as a function of J'/t or V/t in (a) and δ in (b). The solid lines (dotted lines) are energy levels for the local spin twist $\theta = 0$ ($\theta = \pi$). When we consider one of three perturbations of J'/t , V/t and δ , other two parameters are fixed to zero. The spin gap exists around $E = -8 \sim -4$. In addition, the dimerization gap opens in (b) at the middle of the multiplet.

have checked numerically that small perturbations of δ , J' , and V do not close the spin gap in the $N_{\uparrow} = N_{\downarrow} = 1$ case as shown in Fig. 3. The itinerant singlet gives uniformly π Berry phase as shown in the wide class of the t - J models. It should be noted that the dimerization gap opens in the middle of the multiplet in the dimerized t - J chain and the Berry phase of states below the dimerization gap shows the simple alternation of π 's and zeros: $\gamma = \pi$ (or 0) on a link with the strong (or weak) exchange. The Berry phase gives clear classification of the two topologically different phases for the dimerized t - J chain as well as for the dimerized Heisenberg chain.¹³ The differences are (i) the Berry phase in the present paper is that for the multiplet and (ii) the Berry phases of states below the spin gap are π uniformly.

Let us again consider the $N_{\uparrow} = N_{\downarrow} \geq 1$ case in the simple t - J chain. In the large J/t limit, the system is in the phase-separated phase and all the electrons form a Heisenberg chain island.²⁵ The length of the island is $N = N_{\uparrow} + N_{\downarrow}$ and the translation of this island generates L -fold degenerate states. The Berry phase of each degenerate state is obtained from that in the Heisenberg chain. Note that the Berry phases of the Heisenberg chain with even N sites under the open boundary condition turn out to be π on the left and right boundaries and show the simple alternation of π 's and zeros on the other links as mentioned in the dimerized case. After the summation of respective Berry phases of L -fold degenerate states, it follows that the Berry phase of the L -fold multiplet in large J/t limit for $N_{\uparrow} = N_{\downarrow} = N/2$ and $L > 2N$ is uniformly π on every links when $N = 4n + 2$. It is uniformly zero when $N = 4n$, ($n = 0, 1, 2, \dots$). The perturbation with H_t lifts the degeneracy of the large J/t limit. However, the texture pattern of the Berry phases is protected until the spin gap closes. This is numerically confirmed for various L at fixed N in the low density limit. Note that the spin gap closes at finite filling, i.e. infinite N at fixed N/L , which is the case of usual phase separation in the 1D t - J model.

In conclusion, quantized Berry phase as a local order parameter has been calculated in

the t - J models. Comparing the previous study in Heisenberg models,^{12,13} there are gapless charge excitations below the finite spin gap which exists in the large J/t case. Even if the number of states below the gap is large, the Berry phase has been obtained by the exact diagonalization method and Eq. (4) successfully. As a result in the t - J models, the Berry phase for the itinerant singlet is uniformly π on nearest-neighbor links in the 1D and 2D cases. The itinerant singlet carries the Berry phase π in addition to charge, while the singlet does not carry spin. Due to the topological stability of the quantized Berry phase, the picture of the itinerant singlet obtained in the present study (for large J) has been valid in the wide class of t - J models until the spin gap closes. The 1D t - J model has the uniform Berry phase π for the L -fold multiplet below the spin gap especially when the number of electrons N is $4n + 2$.

Moreover, the dimerized t - J model has been classified by a texture pattern of the Berry phases in regard to the dimerization gap. In general, the Berry phase can be defined for each gap and are protected until the gap closing. This method will be useful even for the frustrated electron system. The texture pattern of the Berry phases can be used to find a path to a simple strong limit without gap closing as the results shown in the present paper have the corresponding strong limits. These strong limits tell us the topological property of the phase by using the adiabatic continuity.

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References

- 1) X. G. Wen: Int. J. Mod. Phys. B **5** (1991) 1641.
- 2) Y. Hatsugai: Phys. Rev. Lett. **71** (1993) 3697.
- 3) Y. Hatsugai: J. Phys. Soc. Jpn. **73** (2004) 2604.
- 4) Y. Hatsugai: J. Phys. Soc. Jpn. **74** (2005) 1374.
- 5) F. D. M. Haldane: Phys. Lett. A **93** (1983) 464.
- 6) I. Affleck, T. Kennedy, E. H. Lieb, and H. Tasaki: Phys. Rev. Lett. **59** (1987) 799.
- 7) N. Read and S. Sachdev: Phys. Rev. Lett. **62** (1989) 1694.
- 8) G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev: Phys. Rev. Lett. **90** (2003) 227902.
- 9) T. Hirano and Y. Hatsugai: J. Phys. Soc. Jpn. **76** (2007) 074603.
- 10) H. Katsura, T. Hirano and Y. Hatsugai: Phys. Rev. B **76** (2007) 012401.
- 11) X. G. Wen: Phys. Rev. B **40** (1989) 7387.
- 12) Y. Hatsugai: J. Phys. Soc. Jpn. **75** (2006) 123601.
- 13) Y. Hatsugai: J. Phys.: Condens. Matter **19** (2007) 145209.
- 14) A. A. Aligia: Europhys. Lett. **45** (1999) 411.
- 15) P. Anderson: Science **235** (1987) 1196.
- 16) F. C. Zhang and T. M. Rice: Phys. Rev. B **37** (1988) 3759.
- 17) P. W. Anderson: Phys. Rev. Lett. **64** (1990) 1839.
- 18) E. Dagotto and T. M. Rice: Science **271** (1996) 618.
- 19) F. Wilczek and A. Zee: Phys. Rev. Lett. **52** (1984) 2111.
- 20) R. D. King-Smith and D. Vanderbilt: Phys. Rev. B **47** (1993) 1651.
- 21) D. S. Rokhsar and S. A. Kivelson: Phys. Rev. Lett. **61** (1988) 2376.
- 22) M. Imada: Phys. Rev. B **48** (1993) 550.
- 23) M. Ogata, M. U. Luchini, and T. M. Rice: Phys. Rev. B **44** (1991) 12083.
- 24) M. Troyer, H. Tsunetsugu, T. M. Rice, J. Riera, and E. Dagotto: Phys. Rev. B **48** (1993) 4002.
- 25) M. Ogata, M. U. Luchini, S. Sorella, and F. F. Assaad: Phys. Rev. Lett. **66** (1991) 2388.

